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Critical exponents of the three-dimensional classical plane rotator model on the sc lattice from a high temperature series analysis

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High temperature series expansions of the spin-spin correlation function for the plane rotator (or XY) model on the sc lattice are extended by three terms through order β^{17} . Tables of the expansion coefficients are reported for the correlation function spherical moments of order $l = 0, 1, 2$. Our analysis of the series leads to fairly accurate estimates of the critical parameters.

In three dimensions the two-component vector model is the simplest spin model in the universality class of the superfluid λ transition of ^4He , and of the ferromagnetic transition of magnets with an easy magnetization plane [1]. No high temperature (HT) series studies of this model have appeared in the last two decades in spite of remarkable experimental measurements of the critical parameters in superfluid ^4He and intense theoretical activity in Renormalization Group calculations and by direct Monte Carlo simulations.

In particular we should mention that the critical index ν , which describes the leading singularity of the superfluid fraction in ^4He near the superfluid transition temperature, has been measured with high precision in a long series of experiments by G. Ahlers and his collaborators [2]. As stressed by Ahlers, the superfluid fraction is the most accurately known singular parameter at a critical point, and correspondingly ν is the most accurately known critical index. The most recent experiments yield the value $\nu = 0.6705 \pm 0.0006$.

Unfortunately the critical exponent γ cannot be measured in liquid ^4He and, as far as magnetic systems are concerned, no precise measurements exist either for γ or for ν . A review of static critical properties of ^4He can be found in Ref. [3] and a general discussion of the interpretation of the measurements on ^4He in connection with the problem of confluent singularities is given in Ref. [4].

The Hamiltonian of the three-dimensional plane rotator (or XY) model is

$$H\{s\} = - \sum_x \sum_{\mu=1,3} s(x) \cdot s(x + e_\mu). \quad (1)$$

Here $s(x)$ is a two-component classical spin of unit length associated to the site with position vector $x = n_1 e_1 + n_2 e_2 + n_3 e_3 = (n_1, n_2, n_3)$ of a 3-dimensional simple cubic lattice and e_1, e_2, e_3 are the elementary lattice vectors. The sum over x extends to all lattice sites.

It has been rigorously proved that the model exhibits a ferromagnetic phase transition [5].

We present here series which extend by three terms, to order β^{17} , the series of Ref. [6]. They have been computed by a FORTRAN code which iteratively solves the Schwinger-Dyson equations for the correlation functions [7].

We have tabulated the HTE coefficients of the two-point correlation function

$$C(x; \beta) = \langle s(0) \cdot s(x) \rangle \quad (2)$$

for all inequivalent sites x for which the expansion is non trivial to order β^{17} .

We have analyzed the series for the spherical moments of the correlation function $m^{(l)}(\beta)$ defined as follows:

$$m^{(l)}(\beta) = \sum_x |x|^l C(x; \beta) = \sum_{r=1}^{\infty} a_r^{(l)} \beta^r, \quad (3)$$

(here $|x| = \sqrt{n_1^2 + n_2^2 + n_3^2}$), $l \geq 0$ and the sum extends over all lattice sites. The zeroth order spherical moment $m^{(0)}(\beta)$ is the (reduced) susceptibility and is also denoted by $\chi(\beta)$.

In Table I, we report the HTE coefficients of the spin-spin correlation function $\langle s(0) \cdot s(x) \rangle$ with $x = (1, 0, 0)$.

In Tables II, III and IV we report the expansion coefficients for the moments $m^{(l)}(\beta)$ with $l = 0, 1$ and 2.

Our analysis of this O(2) symmetric model parallels that of the corresponding series for the O(0) symmetric self-avoiding walk (s.a.w.) model and the O(1) symmetric Ising model on the s.c. lattice [[9]]. Using both first-order and second-order differential approximants, we first analyse the susceptibility series. We find that if the degree of the inhomogeneous polynomial is too low (≤ 3) the approximants cannot adequately accommodate the analytic background term. On the other hand if the degree of the inhomogeneous polynomial is too large (≥ 8), there are insufficient series terms to adequately represent the singular part of the series. For intermediate values of the degree of the inhomogeneous polynomial however, the approximants are stable, allowing the unbiased estimates $\beta_c = 0.45406 \pm 0.00005$, $\gamma = 1.315 \pm 0.009$ to be made. The unbiased estimates from second-order approximants were more erratic, giving $\beta_c = 0.4541 \pm 0.0001$, $\gamma = 1.32 \pm 0.01$. Biasing the approximants at $\beta_c = 0.45406$ gave $\gamma = 1.315 \pm 0.005$ and $\gamma = 1.316 \pm 0.005$ from first-order and second-order approximants respectively. The results remain essentially unchanged using either the Fisher-Au Yang/Hunter-Baker definition (no regular singular point at the origin) or the Guttman/Joyce definition of the DAs (a regular singular point at the origin), the difference being mostly in the dispersion of the data (in particular of the background), which is somewhat greater with the former definition.

A similar analysis of the first moment, $m^{(1)}(\beta)$ is less satisfactory. Most of the approximants are defective, but the few that are not are centred around a slightly lower temperature, $\beta_c = 0.4542 \pm 0.0003$, with exponent $\gamma + \nu = 2.00 \pm 0.03$. Biasing the approximants at $\beta_c = 0.45406$ gives mainly defective approximants, slowly decreasing in value, so that we can only estimate $\gamma + \nu \leq 2.00$. The second correlation moment series $m^{(2)}(\beta)$ is somewhat better behaved, though, like the analogous s.a.w. and Ising series, unbiased approximants at first glance give a lower critical temperature than do the susceptibility series approximants, notably $\beta_c = 0.4542 \pm 0.0002$, and $\gamma + 2\nu = 2.69 \pm 0.02$. This behaviour of the series $m^{(2)}(\beta)$ was also noted for the Ising and s.a.w. model series [[9]]. It appears that longer series are needed for higher moments of the correlation function. Biasing the second-moment series at $\beta_c = 0.45406$ gives $\gamma + 2\nu = 2.67$, but this must be regarded as an upper bound as the sequence of estimates of $\gamma + 2\nu$ decreases with increasing numbers of terms - just as observed previously for the corresponding Ising series. While it is difficult to extrapolate this slowly declining sequence, the limit $2.66_{-0.02}^{+0.01}$ is likely sufficiently conservative to include the correct value. In reaching this conclusion we have not only extrapolated this sequence, but have studied the behaviour of analogous sequences for the Ising and s.a.w. model, where we also have exact results for the two-dimensional models to guide us. If this estimate is accepted, we find from our earlier estimate of γ that $\nu = 0.67 \pm 0.01$.

We may also construct the series with coefficients $c_r = m_r^{(2)}/m_r^{(0)}$ and study its singularity at $z = 1$ which should have exponent $2\nu + 1$. Then we get $\nu = 0.68 \pm 0.01$, with again a decreasing sequence of exponent estimates, suggesting that ν is in fact a little lower.

In conclusion our estimates of γ are fairly precise and, as shown later, in good agreement with the Renormalization Group (RG) results. However our estimates of ν cannot yet compete either with the precision of the experimental data nor with the RG or Monte Carlo determinations, although they are perfectly compatible with both. This is probably due to the slow convergence of $m^{(2)}(\beta)$, and as noted above, has already been observed in the study of high order expansions for the SAW and Ising models [[9]]. Longer series are then required in order to make a more accurate analysis possible and in particular to account properly for the confluent singularities.

Let us now briefly review previous high temperature series analyses, restricting our review to the sc lattice results.

Bowers and Joyce [[10]], computed series to order β^8 and gave the following estimates: $\beta_c = 0.4530 \pm 0.0016$, and $\gamma = 1.312 \pm 0.006$.

In Ref. [[11]] the series were extended to order β^{11} . The estimated inverse critical temperature was $\beta_c = 0.4539 \pm 0.0013$ and the corresponding estimates for γ and ν were $\gamma = 1.32 \pm 0.05$ and $\nu = 0.675 \pm 0.015$. A comparison with our results shows that our central values for β_c and γ are significantly lower and that the precision in our estimates has improved by a factor two.

Reliable Monte Carlo simulations with good statistical accuracy, on reasonably sized lattices, have become possible only recently after the invention of algorithms with reduced critical slowing down [[12]]. The largest accurately studied lattice is still only 64^3 sites large (present practical limits seem to be around 100^3 sites), which means that a very accurate treatment of finite size effects is required and that the estimate of systematic errors is very delicate. The oldest analysis is due to Li and Teitel [[13]] who performed a Metropolis simulation (supplemented by over-relaxation method) on lattices up to 16^3 sites. A finite size scaling analysis of their data yields $\beta_c = 0.4533 \pm 0.0006$

and $\nu = 0.67 \pm 0.02$. (The model actually simulated is a clock model with 512 states.)

More recently Hasenbusch and Meyer [[14]] used the Wolff single cluster algorithm on lattices up to 96^3 sites. From a fit of the data to $\chi \propto (\beta_c - \beta)^{-\gamma}$, they found $\beta_c = 0.45421 \pm 0.00008$ and $\gamma = 1.327 \pm 0.008$. A recent update [[15]] of this study using the Wolff single cluster algorithm on lattices up to 64^3 sites gave $\beta_c = 0.45420 \pm 0.00002$, $\nu = 0.664 \pm 0.006$ and $\gamma = 1.324 \pm 0.001$.

W. Janke [[16]] also used the Wolff single cluster algorithm on lattices up to 48^3 sites. From a study of the fourth order cumulant he obtained $\beta_c = 0.4542 \pm 0.0001$ and $\nu = 0.670 \pm 0.002$. Fitting data to the formula $\chi \propto \chi_+(\beta_c - \beta)^{-\gamma}$ he obtained $\beta_c = 0.45408 \pm 0.00008$, and $\gamma = 1.316 \pm 0.005$. Repeating his fit with fixed $\beta_c = 0.4542$ the value of γ increases to $\gamma = 1.323 \pm 0.002$.

The previous computations should also be compared to the estimates by the Renormalization Group applied to an $O(2)$ symmetric ϕ^4 field theory model.

Sixth order perturbation expansion in three dimensions by Baker, Nickel and Meiron [[19]], gave $\gamma = 1.316 \pm 0.009$ and $\nu = 0.669 \pm 0.003$. Subsequently, taking into account the large order behavior of the perturbation series coefficients, Le Guillou and Zinn Justin [[20]] refined these estimates and obtained $\gamma = 1.316 \pm 0.0025$ and $\nu = 0.6695 \pm 0.001$.

Performing the computation [[21]] by the Wilson-Fisher $\epsilon = 4 - d$ expansion Borel resummed to order ϵ^5 , Le Guillou and Zinn Justin subsequently obtained the following estimates: $\gamma = 1.315 \pm 0.007$ and $\nu = 0.671 \pm 0.005$.

It thus appears that the RG results for γ are slightly smaller than the old HT and some of the new Monte Carlo estimates, but perfectly compatible with the results of our analysis, while our estimate of ν is compatible with, but less accurate than, the most recent RG results.

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TABLE I. HTE coefficients of the nearest neighbor correlation $C(0, x)$ with $x = (1, 0, 0)$

order	coefficient
1	0.50000000000000000000000000000000
3	0.43750000000000000000000000000000
5	1.01041666666666666666666666666667
7	2.49169921875000000000000000000000
9	7.48240559895833333333333333333333
11	24.7292479338469328703703703703704
13	86.7042412409706721230158730158730
15	317.800753506891941898083560681217
17	1205.06602454131493586174488161069

TABLE II. HTE coefficients of the susceptibility $m^{(0)}$.

order	coefficient
0	1.00000000000000000000000000000000
1	3.00000000000000000000000000000000
2	7.50000000000000000000000000000000
3	18.37500000000000000000000000000000
4	43.50000000000000000000000000000000
5	102.3437500000000000000000000000000
6	237.0546875000000000000000000000000
7	546.9462890625000000000000000000000
8	1252.0048828125000000000000000000000
9	2858.8175292968750000000000000000000
10	6496.1514078776041666666666666666666
11	14735.37464124891493055555555555555
12	33314.75377468532986111111111111111
13	75222.2566392081124441964285714286
14	169444.488235923222133091517857143
15	381306.311343971793613736591641865
16	856543.263379992410619422872230489
17	1922537.91945074856684251367029620

TABLE III. HTE coefficients of the first correlation moment $m^{(1)}$.

order	coefficient
0	0.00000000000000000000000000000000
1	3.00000000000000000000000000000000
2	11.4852813742385702928101323452582
3	35.3919166429113710288472410676167
4	100.391645797382835211177404733391
5	270.169140885332810622174619548742
6	703.928165009702962171567107355945
7	1789.19653133764917963889959830865
8	4468.32789180460469625866305929854
9	11000.8726669685811734428842857616
10	26788.0560947846126416923232831814
11	64627.3429637161982839763298977200
12	154749.818273239775925845196634614
13	368132.797893714045088109726930470
14	870977.871997489895140365839695762
15	2050710.75491296809029207572988208
16	4808405.28831745065018387682551317
17	11232374.4966970585972846903939187

TABLE IV. HTE coefficients of the second correlation moment $m^{(2)}$.

order	coefficient
0	0.00000000000000000000000000000000
1	3.00000000000000000000000000000000
2	18.00000000000000000000000000000000
3	72.37500000000000000000000000000000
4	247.50000000000000000000000000000000
5	770.59375000000000000000000000000000
6	2261.34375000000000000000000000000000
7	6360.66503906250000000000000000000000
8	17343.77734375000000000000000000000000
9	46158.42104492187500000000000000000000
10	120515.319303385416666666666666666667
11	309746.4250318739149305555555555556
12	785831.296427408854166666666666666667
13	1971809.99205790928431919642857143
14	4901417.59164962163047185019841270
15	12084656.3170853394364553784567212
16	29584235.7640201335230832377438823
17	71970593.8709586784015817546900548